2,3,6-Trifluoroacetophenone

Inchi: InChI=1S/C8H5F3O/c1-4(12)7-5(9)2-3-6(10)8(7)11/h2-3H,1H3
InchiKey: INDGVPJYDRJJPJ-UHFFFAOYSA-N
Formula: C8H5F3O
SMILES: CC(=O)c1c(F)ccc(F)c1F
Mol. weight [g/mol]: 174.12
CAS: 208173-22-2

Physical Properties

Property code	Value	Unit	Source
gf	-613.35	kJ/mol	Joback Method
hf	-707.24	kJ/mol	Joback Method
hfus	20.19	kJ/mol	Joback Method
hvap	41.96	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.307		Crippen Method
mcvol	106.700	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
tb	475.74	K	Joback Method
tc	668.03	K	Joback Method
tf	295.60	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.71	J/mol×K	475.74	Joback Method
cpg	226.59	J/mol×K	507.79	Joback Method
cpg	235.05	J/mol×K	539.84	Joback Method
cpg	243.09	J/mol×K	571.88	Joback Method
cpg	250.73	J/mol×K	603.93	Joback Method
cpg	257.96	J/mol×K	635.98	Joback Method
cpg	264.80	J/mol×K	668.03	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C208173222&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume